

3-Hydroxy-4-methoxy-benzaldehyde
621-59-0 | DTXSID7049423

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 1.10

Global applicability domain: Inside

Local applicability domain index: 6.62e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

| | | |
|--|---|---|
| <div>Image not found</div> <div>4-Hydroxy-3-methoxybenzaldehyde</div> <div>Measured: 1.21</div> <div>Predicted: 1.09</div> | <div>Image not found</div> <div>3-Hydroxy-4-methoxybenzaldehyde</div> <div>Measured: 0.97</div> <div>Predicted: 1.10</div> | <div>Image not found</div> <div>3-Ethoxy-4-hydroxybenzaldehyde</div> <div>Measured: 1.58</div> <div>Predicted: 9.56e-01</div> |
| <div>Image not found</div> <div>1,3-Benzodioxole-5-methanol</div> <div>Measured: 1.05</div> <div>Predicted: 3.86e-01</div> | <div>Image not found</div> <div>2-Ethyl-3-hydroxy-4H-pyran-4-one</div> <div>Measured: 0.63</div> <div>Predicted: 4.56e-01</div> | |